Yang Li

Scientist, Data Science,

Global Health Drug Discovery Institute

Email: Yang.li@ghddi.org

Website: https://yangli59.github.io/

ResearchGate: https://www.researchgate.net/profile/Yang-Li-802

Strength Summary

- Pharmaceutical scientist with a PhD and experience in computer-aided drug design.
- Expertise in drug screening strategies and structure modification.
- Experience in building QSAR models, protein-ligand docking, protein-protein docking, binding free energy prediction, and drug likeness prediction.
- Experienced in computational biology: Engaged in the construction of multiscale models for complex systems and multiscale molecular dynamics simulations to explain the mechanisms of molecular recognition and dissociation between molecules.
- Experience with all-atom molecular dynamics simulations, coarse-grained molecular dynamics simulations, metadynamics, umbrella sampling, Gaussian accelerated sampling in molecular dynamics simulations, analysis of molecular interaction networks, and free energy landscape calculations.
- Focus on the development of new molecular dynamics methods with advanced sampling , adept at the application of target prediction tools for small molecules, and peptide-based drug development.

Education

- 2017.9 – 2020.7 | Ph.D. | Pharmaceutical chemistry | Nankai University
  Supervisor: Prof. Jianping Lin
- 2014.7 – 2017.9 | Master | Pharmaceutical chemistry | Nankai University
- 2009.9 – 2013.7 | Bachelor | Pharmacy | China Pharmaceutical University

Professional Experience

2023.7 – Present **Global Health Drug Discovery Institute**
Scientist, Data Science

- Supporting biologists and chemists in preliminary drug screening and structural modifications.
- Promote structure prediction, virtual screening and hit selection, and support hit-to-lead optimization and balance between potency and ADME properties.
- Deeper understanding of diseases caused by respiratory viruses and their targets.
- Assemble MD workflows to perform automated MD calculations and develop strategies that link structural features to potency or resistance.

2020.6 – 2023.6 **Nankai University**

Postdoctoral Fellow with Prof. Yuequan Shen (Prof. Shen is the Chief Scientist of 973 project).

- Investigation of the molecular basis of Mg2+ permeation through the human mitochondrial Mrs2 channel by umbra sampling method
- Develop a new advanced sampling molecular dynamics method called Su-GaMD simulations and visualise the activation mechanism of the adenosine A1 receptor.
- Investigate the self-organisation of the heptameric/octameric calcium homeostasis modulator 1 channel.
- Modelling the pore opening of the human TACAN after application of mimetic force.

Publications/ Research Achievements

- Li, Ming[#], **Yang Li[#]**, Yue Lu, Jianhui Li, Xuhang Lu, Yue Ren, Tianlei Wen, *Yaojie Wang, Shenghai Chang, Xing Zhang, Xue Yang[*], Yuequan Shen[*].*, Molecular Basis of Mg2+ Permeation through the Human Mitochondrial Mrs2 Channel. *Nature Communications,* **2023**, 14, 1 4713.

- **Yang Li[#]**, Jixue Sun[#], Dongmei Li[*], Jianping Lin[*]., The full activation mechamism of adenosine A_1 receptor revealed by GaMD and supervised GaMD (Su-GaMD) simulations., *Proceedings of the National Academy of Sciences of the United States of America*, **2022**, 119, 42, e2203702119.
- Yue Ren[#], **Yang Li[#]**, Yaojie Wang, Tianlei Wen, Xuhang Lu, Shenghai Chang, Xing Zhang, Yuequan Shen[*], XueYang[*]., Cryo-EM structure of the heptameric calcium homeostasis modulator 1 channel., *Journal of Biological Chemistry,* **2022**: 101838.

- Xiaozhe Chen[#], Yaojie Wang[#], **Yang Li[#]**, Xuhang Lu, Jianan Chen, Ming Li, Tianlei Wen, Ning Liu, Shenghai Chang, Xing Zhang, Xue Yang[*], Yuequan Shen[*], Cryo-EM structure of the human TACAN in a closed state., *Cell Reports*, **2022**, 38 (9), 110445.

- **Yang Li**, XueYang[*], Yuequan Shen[*], Structural insights into Ca2+ permeation through Orai channels., *Cells,* **2021**: 10 (11), 3602.
- **Yang Li**, Mukuo Wang, Na Gao, Dongmei Li[*], Jianping Lin[*], The effect of dimerization on the activation and conformational dynamics of adenosine A_1 receptor., *Physical Chemistry Chemical Physics*, **2019**, 21 (41), 22763-22773.
- Yu Wei[#], Mukuo Wang[#], **Yang Li[#]**, Zhangyong Hong, Dongmei Li[*], Jianping Lin[*], Identification of new potent A_1 adenosine receptor antagonists using a multistage virtual screening approach., *European Journal of Medicinal Chemistry*, **2019**, 187, 111936.
- **Yang Li[#]**, Can Yin[#], Pi Liu[#], Dongmei Li[*], Jianping Lin[*], Identification of a different agonist-binding site and activation mechanism of the human $P2Y_1$ receptor., *Scientific Reports*, **2017**, 7: 13764.
- **Yang Li**, Jixue Sun, Dongmei Li[*], Jianping Lin[*], Activation and conformational dynamics of a class B G-protein-coupled glucagon receptor., *Physical Chemistry Chemical Physics*, **2016**, 18, 12642-12650.

Certificate

Certification by the China Postdoctoral Science Foundation (Grant No. BSMS69004)